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# Enhancing the Plausibility of Law Equation Discovery

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## Abstract

After the pioneering work of the BACON system, the study in the field of scientific discovery has been directed to the discovery of more plausible law equations to represent the first principles underlying objective systems. The state of the art has only succeeded in a weak sense that the soundness, the reproducibility and the mathematical admissibility of the candidates hold within the experimental measurements. The plausibility should be checked for various objects and/or measurements sharing the common first principles, and only the equations having sufficient generality should be retained. In this paper, a novel principle and an algorithm are proposed to predict some mathematically admissible and consistent equation formulae for a newly given set of quantities from the candidate law equations obtained for another set of quantities in advance. The soundness and the reproducibility of the predicted equations are confirmed through the measurements. The law equations which passed all confirmations represent the common first principles under different set of quantities.

## 1. Introduction

The main goal of the scientific law equation discovery is to discover the first principle based law equations from measurement data. The most well known pioneering system to discover scientific law equations under the condition where some quantities are actively controlled in a laboratory experiment is BACON (Langley et al., 1987). FAHRENHEIT (Koehn & Zytkow, 1986) and ABACUS (Falkenhainer, & Michalski, 1986) are successors that basically use similar algorithms to BACON to discover law equations. LAGRANGE

(Dzeroski & Todorovski, 1995) is another type of scientific law equation discovery systems based on the ILP-like generate and test reasoning to discover equations representing the dynamics of the objects.

To reduce the ambiguity in their results under noisy measurements and the high computational cost of their algorithms, some subsequent discovery systems, *e.g.*, FAHRENHEIT, ABACUS and COPER (Kokar, 1986), introduced the use of the unit dimension of physical quantities to prune the meaningless solutions. A difficulty of this approach is its narrow applicability only to the quantities whose units are clearly known. The recently proposed system named SDS has overcome these difficulties (Washio & Motoda, 1997, 1998). It discovers scientific law equations by limiting its search space to mathematically admissible equations in terms of the constraints of *scale-type* and *identity*. Since the knowledge of scale-types is widely obtained in various domains, SDS is applicable to non-physical domains including biology, sociology, and economics.

The framework has been further extended to the passively observed data where any active control on quantities are not admitted. Aforementioned FAHRENHEIT has a function to discover law equations from the observed data. LAGRANGE can handle this task in its generate and test framework. More recently, SDS has been also extended to this task (Washio et al., 1999). Its excellent features of the robustness against observation noise and the limited computational complexity have been demonstrated.

In spite of these efforts, the state of the art is that the techniques has only succeeded in discovering the plausible candidates of law equations in a weak sense that the soundness, the reproducibility and the mathematical admissibility of the candidates hold within a given experimental environment. However, a law equation should hold over various objects and/or measurements sharing the common first principles. Accord-

ingly, the *generality* of the candidate equations should be assessed under various environments so as to retain only highly plausible law equations in a strong sense.

More strictly speaking, two types of generality should be considered. One is the generality of the law equation over multiple objects sharing some identical first principles. Another is the generality over multiple combinations of measurement quantities. The first generality is explained through the following example of Kepler's third law,

$$\frac{T^2}{a^3} = C, \quad (1)$$

where  $T$  is the period of revolution,  $a$  the major radius of elliptic orbit, and  $C$  a constant. It has the generality over multiple planets. Given an experimental or observation environment, the current law equation discovery systems can figure out the generality of this equation only limited to the given objects such as the planets in the solar system. The automatic generalization of the equation for wider domains such as every pair of mass points in a free space is beyond the scope of the current research field.

The second generality is demonstrated through the following irregular expression of Kepler's laws for any elliptic orbits having a certain eccentricity,

$$T^4 \dot{\omega}_a^3 = C', \quad (2)$$

where  $\dot{\omega}_a$  is the angular velocity of the planet on the major axis of the elliptic orbit and  $C'$  a constant. Kepler initially discovered this type of law equations because the distance information on the planet orbits was hardly obtained. Later, he generalized Eq.(2) into Eq.(1) in concert with the following his second law,

$$\dot{S} = \frac{r^2 \dot{\omega}}{2} = C'', \quad (3)$$

where  $\dot{S}$  is the areal velocity,  $r$  the distance between the sun and the planet,  $\dot{\omega}$  the angular velocity of the planet and  $C''$  a constant. Both Eq.(1) and Eq.(2) are the relations associated with the period of revolution under the different combinations of measurement quantities. Because the consistency between the two equations are ensured by Eq.(3), these two equations are considered to represent a unique first principle and show the second generality.

The objectives of this paper are:

1. to propose a principle to reason some mathematically admissible and consistent law equation formulae for a newly given set of quantities based on

the candidate law equation formulae discovered from another set of quantities and their measurement data in advance,

2. to propose an algorithm to predict mathematically admissible and consistent law equation formulae by the above principle and to check the plausibility of the candidate law equations in terms of the second generality, i.e., if the predicted formulae are well supported by the measurement of the newly given set of quantities, and
3. to evaluate and demonstrate the practicality of the proposed algorithm through a real world scientific law discovery in socio-psychology.

When two candidate law equations are independently discovered by a law equation discovery system from two different sets of measurement quantities  $Q_s$  and  $Q_t$ , their mutual second generality can be assessed by checking the consistency between the two candidates based on the proposed principle. However, the algorithm proposed in this study predicts law equation formulae for  $Q_t$  from the candidate law equation for  $Q_s$ , and check if the predicted formula explains the data of  $Q_t$ . This approach has the following advantages:

- A. Amount of data and reasoning cost required to check the applicability of the predicted formulae to the measurement data of  $Q_t$  are much less compared with those needed to apply the law equation discovery system to the data of  $Q_t$ .
- B. The applicability checking of the predicted formulae to  $Q_t$  is more robust against the noise than the case to derive candidate law equations for  $Q_t$  by using the law equation discovery system.
- C. Complex but admissible law equations which may be missed by some conventional law equation discovery systems can be discovered.

These advantages are demonstrated through the performance evaluation and the practical application of the proposed approach in this paper.

## 2. Scale-type Constraints

The background theory of the proposing principle is provided by the scale-types of measurement quantities and the constraints on the admissible relations of pair wise quantities associated with the scale-types. The discussion on the scale-types was given by Stevens (1946). He mathematically characterized and categorized quantitative quantities into two major scale-types of interval scale and ratio scale. Examples of

the interval scale quantities are temperature in Celsius and sound tone where the origins of their scales are not absolute, and are changeable by human's definitions. Its admissible unit conversion follows "*Generic linear group*:  $x' = kx + c$ ". Examples of the ratio scale quantities are physical mass and absolute temperature where each has an absolute zero point. Its admissible unit conversion follows "*Similarity group*:  $x' = kx$ ".

Luce (1959) claimed that the basic formula of the functional relation among quantities of ratio and interval scales can be determined by their scale-type features, if the quantities have direct dependency without being coupled through any dimensionless quantities. Under this condition, some unit dimensions of the quantities are related to each other, and consequently the unit change of a quantity affects the value of other quantity. Suppose  $x_i$  and  $x_j$  are both ratio scale quantities, and  $x_i$  is defined by  $x_j$  through a logarithmic functional relation  $x_i = u(x_j)$ , *i.e.*,  $x_i = \log x_j$ . We multiply a positive constant  $k$  to  $x_j$ , *i.e.*, a change of unit, without violating the group structure of the ratio scale quantity  $x_j$ , then this leads  $u(kx_j) = \log k + \log x_j$ . This fact causes the shift of the origin of  $x_i$  by  $\log k$ , and violates the group structure of  $x_i$  which is the ratio scale quantity. Hence, the direct functional relation from  $x_j$  to  $x_i$  must not be logarithmic. As the admissible transformations of  $x_i$  and  $x_j$  in their group structures are  $x'_i = Kx_i$  and  $x'_j = kx_j$  respectively, the generic formula of  $x_i = u(x_j)$  must satisfy the invariant condition of  $x'_i = u(x'_j) \leftrightarrow Kx_i = u(kx_j)$  under the unit conversion. The factor  $K$  of the changed unit of  $x_i$  depends on  $k$ , but it shall not depend upon  $x_j$ , so we denote it by  $K(k)$ . Consequently, we obtain the following constraints on the continuous function  $u(x_j)$ ,

$$u(kx_j) = K(k)u(x_j),$$

where  $k > 0$  and  $K(k) > 0$  as these are the factors of the unit change. The constraints for all combinations of the scale types are summarized in Table 1. Luce (1959) derived each solution of  $u(x_j)$  under the condition of  $x_j \geq 0$  and  $u(x_j) \geq 0$ . We have extended his theory to cover the negative values of  $x$  and  $u(x_j)$  (Washio & Motoda, 1996). The generic solution of  $u(x_j)$  in each case is summarized in Table 2. The impossibility of the definition of a ratio scale from an interval scale is because the ratio scale involves the information of an absolute origin, but the interval scale does not. In this table, the inverse functions of the cases 2.1 and 2.2 are listed at 3.1 and 3.2 for use in the algorithm shown in the next section.

### 3. Principle and Algorithm

Let  $Q_s$  be a source set of measurement quantities, and  $\psi_s = 0$  a source equation where all of its arguments belong to  $Q_s$ . Furthermore, let  $\delta_{ij}$  be an operator to commute a quantity  $x_i$  to another  $x_j$  in a set of quantities, and  $\delta_{ij}\psi = 0$  an equation where the argument  $x_i$  is changed to  $x_j$  in  $\psi = 0$  by substituting the relation  $x_i = u(x_j)$ . Our task is to derive a set of the admissible target equation  $E_t = \{\psi_{tk} = 0, k = 1, \dots, m\}$  from the source equation  $\psi_s = 0$  where all arguments of each  $\psi_{tk} = 0$  belong to a target set of measurement quantities  $Q_t$ .  $Q_t$  is derived from  $Q_s$  by applying a set of the commutation operators  $\Delta_{st} = \{\delta_{ij} | x_i \in Q_s, x_j \in Q_t\}$ , and thus the cardinality of  $Q_t$  is equal to that of  $Q_s$ .

If  $\psi = 0$  and  $x_i = u(x_j)$  is known in a priori, then the equation formula  $\delta_{ij}\psi = 0$  is easily derived. However, our interest is to derive  $\delta_{ij}\psi = 0$  when  $x_i = u(x_j)$  is unknown in advance. In this paper, the situation, where the following two assumptions hold, is considered.

**Assumption 1** *The scale types of the quantities for commutations are known.*

**Assumption 2** *The quantities  $x_i$  and  $x_j$  have direct dependency without being coupled through any dimensionless quantities.*

The first assumption does not yield any strong limitations since the scale-types of measurement quantities are widely known (Washio & Motoda, 1997). The second assumption holds, when  $x_i$  and  $x_j$  are the quantities to measure an identical feature through different processes and/or when they are known to have direct dependency based on the background knowledge in the domain as for the case of Kepler's laws. This type of quantity pairs are widely seen in various domains as shown later. When the two assumptions hold, some unit dimensions are shared by  $x_i$  and  $x_j$ , and thus the scale-type constraints indicated in Table 2 can be applied. Starting from the source equation  $\psi_s = 0$ , the application of all operators  $\delta_{ij} \in \Delta_{st}$  derives the target equation  $\psi_{tk} = 0$ . In each application of  $\delta_{ij}$ ,  $x_i = u(x_j)$  is selected from Table 2 based on the scale-types of  $x_i$  and  $x_j$ . Multiple solutions of  $\psi_{tk} = 0$  may be derived since both two candidates of  $x_i = u(x_j)$  are applied in case that  $x_i$  and  $x_j$  is the pair of interval and ratio scale quantities. Accordingly, these commutation operations may result in a set of target equations  $E_t$ . In case of a pair of interval and ratio scale quantities, the relations of 2.1 and 2.2 in Table 2 must be used since the interval scale quantity is always defined by the ratio scale quantity. The relations 3.1 and 3.2 which is the inverse of 2.1 and 2.2, must be

Table 1. Constraints on functional relations under scale-type characteristics.

| $C_n$<br>NO. | SCALE TYPES                      |  | CONSTRAINTS*                            | COMMENTS*            |
|--------------|----------------------------------|--|---|----------------------|
|              | INDEPENDENT<br>VARIABLE<br>$x_j$ | DEPENDENT<br>(DEFINED)<br>VARIABLE $x_i$ |   |                      |
| 1            | RATIO                            | RATIO                                    | $u(kx_j) = K(k)u(x_j)$                  | $k > 0, K(k) > 0$    |
| 2            | RATIO                            | INTERVAL                                 | $u(kx_j) = K(k)u(x_j) + C(k)$           | $k > 0, K(k) > 0$    |
| 3            | INTERVAL                         | RATIO                                    | $u(kx_j + c) = K(k, c)u(x_j)$           | $k > 0, K(k, c) > 0$ |
| 4            | INTERVAL                         | INTERVAL                                 | $u(kx_j + c) = K(k, c)u(x_j) + C(k, c)$ | $k > 0, K(k, c) > 0$ |

\*C AND  $\bar{C}$  CAN BE ANY REAL NUMBERS.

Table 2. The admissible relations under scale-type characteristics.

| Eq.<br>NO. | SCALE TYPES                      |  | POSSIBLE RELATIONS                       | COMMENTS*                          |
|------------|----------------------------------|--|--|------------------------------------|
|            | INDEPENDENT<br>VARIABLE<br>$x_j$ | DEPENDENT<br>(DEFINED)<br>VARIABLE $x_i$ |  |                                    |
| 1          | RATIO                            | RATIO                                    | $x_i = \alpha_*  x_j ^\beta$             | $\beta/x_j, \beta/x_i$             |
| 2.1        | RATIO                            | INTERVAL                                 | $x_i = \alpha \log  x_j  + \beta_*$      | $\alpha/x_j$                       |
| 2.2        |                                  |  | $x_i = \alpha_*  x_j ^\beta + \delta$    | $\beta/x_j; \beta/x_i; \delta/x_j$ |
| 3          | INTERVAL                         | RATIO                                    | IMPOSSIBLE                               |                                    |
| 3.1        |                                  |  | $x_i = \alpha_{*a} e^{\beta x_j}$        | $\beta/x_j$                        |
| 3.2        |                                  |  | $x_i = \alpha_{*b}  x_j + \delta ^\beta$ | $\beta/x_j; \beta/x_i; \delta/x_j$ |
| 4          | INTERVAL                         | INTERVAL                                 | $x_i = \alpha_*  x_j  + \beta$           | $\beta/x_j$                        |

- 1) THE NOTATIONS  $\alpha_*, \beta_*$  ARE  $\alpha_+, \beta_+$  FOR  $x_j \geq 0$  AND  $\alpha_-, \beta_-$  FOR  $x_j < 0$ , RESPECTIVELY.
- 2) THE NOTATIONS  $\alpha_{*a}$  IS  $\alpha_+$  FOR  $x_i \geq 0$  AND  $\alpha_-$  FOR  $x_i < 0$ , RESPECTIVELY.
- 3) THE NOTATIONS  $\alpha_{*b}$  IS  $\alpha_{++}$  FOR  $x_i \geq 0, x_j - \delta \geq 0$ ,  $\alpha_{+-}$  FOR  $x_i \geq 0, x_j - \delta < 0$ ,  $\alpha_{-+}$  FOR  $x_i < 0, x_j - \delta \geq 0$ , AND  $\alpha_{--}$  FOR  $x_i < 0, x_j - \delta < 0$ , RESPECTIVELY.
- 4) THE NOTATIONS  $\alpha/x$  MEANS “ $\alpha$  IS INDEPENDENT OF THE UNIT  $x$ ”.
- 5) THE RELATIONS IN 3.1 AND 3.2 ARE NOT DERIVED FROM THEIR CONSTRAINTS, BUT ARE INVERSE FUNCTIONS OF 2.1 AND 2.2.

applied in case to commute a ratio scale quantity to an interval scale quantity.

By using this principle, the algorithm shown in Table. 3 tries to discover the law equation formulae  $\psi_{tk} = 0$  for the target set of measurement quantities  $Q_t$ , and confirms the second generality of the candidate law equations if  $\psi_{tk} = 0$  is checked to be consistent with the measurement data of  $Q_t$ . For a comprehensive explanation, this algorithm is demonstrated through a simple example shown by the aforementioned Kepler’s third law. Let Eq.(2) be a source equation  $\psi_s = 0$ , and consider the case to commute the angular velocity  $\dot{\omega}_a$  to the major radius  $a$  where both are ratio scale. Hence,  $Q_s = \{T, \dot{\omega}_a\}$  and  $Q_t = \{T, a\}$ . In the step (S1), the candidate law equations under  $Q_s$  are discovered by a law equation discovery system such as SDS. In this example, Kepler discovered the candidate law equation Eq.(2).

In the step (S2), the target equation formulae under  $Q_t$  are reasoned through the procedure *REASONING*. In *REASONING*, when  $\Delta$  is not empty, a commutation operator  $\delta_{ij}$  is popped from  $\Delta$ , and  $x_i$  in  $\psi$  is commuted to  $x_j$  by the operator. If  $x_i = u(x_j)$  is one of the cases 2.1, 2.2, 3.1 and 3.2 in Table 2, two candidate formulae are derived, i.e.,  $h = 1, 2$ , otherwise

a unique candidate formula is derived. This procedure is recursively applied to each candidate formula until  $\Delta$  becomes empty. In the example of Eq.(2),  $\dot{\omega}_a = \alpha_* |a|^\beta$  is selected from Table 2 for the commutation in *REASONING* of the step (S2). By substituting this relation to Eq.(2), the following equation formula is predicted,

$$T^4 |a|^{3\beta} = C' \alpha_*^{-3}. \quad (4)$$

Without using the measurement data on  $a$ , the shape of Kepler’s third law is obtained.

Finally, in the step (S3), the least square fitting of the predicted target equations to the measurement data of  $Q_t$  is conducted, and their consistency with the data is assessed. The following statistical *F*-test is used to judge if a target equation shows the consistency with the data of  $Q_t$ . This is the standard *F*-test to judge if the data fitting of an equation is acceptable in statistical sense.

$$\text{If } F_0 > F(d-1, n-d, \alpha) \quad (5)$$

then the fitting is acceptable, else unacceptable,

where

$$V_R = S_R/(d-1), V_e = S_e/(n-d) \text{ and } F_0 = V_R/V_e.$$

Here,  $S_R$  is the regressive component,  $S_e$  the resid-

Table 3. Algorithm to check the generality.

- (S1) Given measurement environments for  $Q_s$ , apply a law equation discovery system to the measurements of  $Q_s$ . Let  $E_s = \{\psi_{sh} = 0, h = 1, \dots, \ell\}$  be the set of discovered candidate law equations.
- (S2) Given  $Q_t$ , and let  $\Delta_{st}$  be a stack of the commutation operators to derive  $Q_t$  from  $Q_s$ .  
 $E_t = \phi$ . For every  $\psi_{sh} = 0 \in E_s$ , {  
 $E_{th} = \phi$ . Apply the procedure  
 $REASONING(\psi_{sh} = 0, \Delta_{st}, E_{th})$   
and obtain the target equation set  
 $E_{th} = \{\psi_{thk} = 0, k = 1, \dots, m_h\}$   
for  $\psi_{sh} = 0$ .  $E_t \leftarrow E_t \cup E_{th}$ .}
- (S3)  $E_f = \phi$ . For every  $\psi_{thk} = 0 \in E_t$  {  
apply the least square fitting of  $\psi_{thk} = 0$   
to the measurements of  $Q_t$ .  
If the goodness of the fitting is accepted  
by  $F$ -test,  $E_f \leftarrow E_f \cup \{\psi_{thk} = 0\}$ .}  
The set of pairs  $E_{st} = \{(\psi_{sh} = 0, \psi_{thk} = 0) | \psi_{thk} = 0 \in E_f\}$  contains highly plausible law equations in terms of the generality.

$REASONING(\psi = 0, \Delta, E_t)$  {

- (P1) If  $\Delta = \phi$ , then  $E_t \leftarrow E_t \cup \{\psi = 0\}$ ,  
and return  $E_t$ .
- (P2) Pop an operator  $\delta_{ij}$  from  $\Delta$ .  
apply  $\delta_{ij}$  to  $\psi = 0$ , and obtain the equation  
set  $E = \{\delta_{ij}^h \psi = 0 | h = 1 \text{ or } 1, 2\}$ .
- (P3) For every equation in  $E$ ,  
apply  $REASONING(\delta_{ij}^h \psi = 0, \Delta, E_t)$ .
- (P4) Push the operator  $\delta_{ij}$  to  $\Delta$ ,  
and return  $\Delta$  and  $E_t$ .}

ual error component,  $d$  the number of measurement quantities in the equation,  $n$  the total number of measurement data used for the fitting and  $F(d-1, n-d, \alpha)$  the lower bound of  $F$  value under the degree of freedom  $(d-1, n-d)$  and  $\alpha$  a risk rate.  $\alpha$  is set to be 0.05 throughout this paper. When the target equation  $\psi_{thk} = 0$  is accepted, both  $\psi_{sh} = 0$  and  $\psi_{thk} = 0$  are considered to have the second type of generality. In the example, the formula Eq.(4) is adopted to the equation fitting on the measurement data  $Q_t = \{T, a\}$  of the planet orbits, and the value of  $\beta$  becomes known to be  $-2$ . The resultant equation involves an absolute value operator  $|\bullet|$  on  $a$ , however, this does not have any essential effect on the relation since the major radius  $a$  is always positive. Thus, Eq.(1) is obtained, and

the mutual generality of Eq.(1) and Eq.(2) has been confirmed. This algorithm can be iteratively applied to achieve higher plausibility of the candidates, if the measurement data of extra  $Q_t$  are available.

Assumption 2 is a sufficient condition that  $x_i$  and  $x_j$  have the relations represented in Table 2, i.e., if they have a direct dependency, then the target law equation formula  $\psi_{thk} = 0$  holds. In other words, if the measurement data of  $Q_t$  do not follow any target law equation formulae, the strong evidence that  $x_i$  and  $x_j$  do not have any direct dependency is provided. Otherwise,  $\psi_{thk} = 0$  can be accepted as a law equation formula for  $Q_t$  as far as it well fits to the measurement data of  $Q_t$ .

#### 4. Performance Evaluation

The basic performance of the proposed method has been evaluated through some simulation examples. One of the major issues of the performance is the noise robustness of the equation fitting and the statistical  $F$ -test to judge if the derived target equation shows the consistency with the data of  $Q_t$ . The second important issue is the performance to identify a correct target equation from the multiple candidate target equations in case that the commutations between the interval and ratio scale quantities are involved. The third important issue is the performance to judge if the commuted quantity  $x_i$  has the direct dependency with  $x_j$ .

Table 4 shows the evaluation result for the four artificial simulation examples. The second column indicates the original candidate law equations which have been discovered in the step (S1) in Table 3. SDS has been used to discover these equations since the scale-types of the quantities are all known in these examples, and the performance of SDS is known to be high from the past experience (Washio & Motoda, 1997, 1998). The third column shows the true formulae of the target equations used in the simulations. The fourth indicates the candidate target equations deduced in the step (S2). The symbols of the constants appearing in Table 2 are retained in these expressions. The fifth shows the equations resulted in the least square fitting in the step (S3). The data of  $Q_t$  was generated through the simulation using the true target equations, and the nonlinear least squares fitting method of Levenberg-Marquardt has been applied (More, 1977). Some constants in the candidate equations have been put together into smaller numbers here. They are represented, only when the equations are accepted by  $F$ -test in the majority of trials. The rest of the columns shows the percentage of the

Table 4. Performance evaluation for simulation examples.

| CASES       | SOURCE                                   | TRUE TARGET  | CANDIDATE  | IDENTIFIED   | F-TEST |      |      |
|-------------|--|--|--|--|--------|------|------|
|             |  |  |  |  | 0%     | 5%   | 20%  |
| KEPLER      | $T = 297.2\omega_a^{-0.75}$              | $T = 5.39 \times 10^{-10} a^{1.5}$                   | $T = 297.2\alpha_*^{-0.75}  a ^{-3/4\beta}$  | $T = 5.67 \times 10^{-10} a^{1.49}$                  | 100%   | 100% | 100% |
| HEAT TRANS. | $\dot{H} = K(T_{c1} - T_{c2})$           | $\dot{H} = K(T_{a1} - T_{a2})$                       | $\dot{H} = K(\alpha_1 \log  T_{a1}  - \alpha_2 \log  T_{a2}  + (\beta_{1*} - \beta_{2*}))$   | $\dot{H} = K(0.993T_{a1} - 0.998T_{a2})$             | 0%     | 0%   | 0%   |
|             |  |  | $\dot{H} = K(\alpha_{1*}  T_{a1} ^{\beta_1} - \alpha_{2*}  T_{a2} ^{\beta_2} + (\delta_1 - \delta_2))$   |  | 100%   | 100% | 100% |
|             |  |  | $\dot{H} = K(\alpha_1 \log  T_{a1}  - \alpha_{2*}  T_{a2} ^{\beta_2} + (\beta_{1*} - \delta_2))$   |  | 0%     | 0%   | 0%   |
|             |  |  | $\dot{H} = K(\alpha_{1*}  T_{a1} ^{\beta_1} - \alpha_2 \log  T_{a2}  + (\delta_1 - \beta_{2*}))$   |  | 0%     | 12%  | 0%   |
| EL. AMP.    | $V_o = \frac{R(1+h_{fe})}{R+R_{BE}} V_i$ | $A_o = A_i + 4.34 \log \frac{R(1+h_{fe})}{R+R_{BE}}$ | $A_o = \frac{\beta_i}{\beta_o} A_i + \frac{1}{\beta_o} \log \left( \frac{\alpha_{i*o}}{\alpha_{o*a}} \frac{R(1+h_{fe})}{R+R_{BE}} \right)$                   | $A_o = A_i + 4.71 \log \frac{R(1+h_{fe})}{R+R_{BE}}$ | 100%   | 100% | 53%  |
|             |  |  | $A_o = \pm \left( \frac{\alpha_{i*b}}{\alpha_{o*b}} \frac{R(1+h_{fe})}{R+R_{BE}} \right)^{1/\beta_o}$  |  | 7%     | 0%   | 0%   |
|             |  |  | $A_o =  A_i + \delta_i ^{\frac{\beta_i}{\beta_o}} - \delta_o$  |  | 0%     | 0%   | 0%   |
|             |  |  | $A_o = \pm \left( \frac{\alpha_{i*a}}{\alpha_{o*b}} \frac{R(1+h_{fe})}{R+R_{BE}} \right)^{1/\beta_o}$  |  | 0%     | 0%   | 0%   |
|             |  |  | $A_o = e^{\frac{\beta_i}{\beta_o} A_i} - \delta_o$   |  | 0%     | 0%   | 0%   |
|             |  |  | $A_o = \frac{\beta_i}{\beta_o} \log  A_i + \delta_i  + \frac{1}{\beta_o} \log \left( \frac{\alpha_{i*b}}{\alpha_{o*a}} \frac{R(1+h_{fe})}{R+R_{BE}} \right)$ |  | 0%     | 0%   | 0%   |
| PENDULUM    | $\dot{x} = A\omega \cos \omega t$        | $\dot{x} = A\omega \cos \arcsin(x/A)$                | $\dot{x} = A\omega \cos \omega \alpha_*  x ^\beta$   |  | 0%     | 0%   | 0%   |

accepted cases for each candidate target equation under 50 measurement data of  $Q_t$  with the noise level of 0%, 5% and 20%. The aforementioned fifth column indicates the equations identified under the 5% noise level. The noise level stands for the standard deviation of the Gaussian random noise relative to the absolute value of each quantity. Totally, 100 trials were conducted for each candidate, and the percentage of the acceptance was calculated.

The first example is the case of the aforementioned Kepler's third law. The candidate target equation has been successfully accepted even under the large noise of 20%. The second is an example of heat transfer across a surface between materials of temperature  $T_{c1}$  and  $T_{c2}$  in Celsius unit which are interval scale.  $K$  is the heat transfer coefficient, and  $\dot{H}$  is the heat transfer rate. In this example, the temperature is commuted to the absolute temperature  $T_{a1}$  and  $T_{a2}$  in Kelvin unit which are ratio scale. Because of the two candidate re-

lations of 2.1 and 2.2 in Table 2 for each commutation, totally four candidate target equations are obtained. The second candidate is the correct one, and it is perfectly accepted by  $F$ -test under any noise levels, while the others are mostly rejected. The target equation has been successfully reconstructed in the equation formula shown in the fifth column. The third example is the relation between the input and the output voltage differences  $V_i$  and  $V_o$  of the electric emitter follower amplifier consisting of a transistor and a resistance.  $R_{BE}$  is the resistance between the base and the emitter of the transistor and  $h_{fe}$  the amplification ratio between the base and the collector electric currents.  $V_i$  and  $V_o$  which are ratio scale become to be represented in form of the logarithmic intensity,  $A_i$  and  $A_o$  in  $dB$  in the target equation. Since  $A_i$  and  $A_o$  are interval scale, again four candidate target equations are deduced, where the first candidate is correct. As shown in the columns of  $F$ -test, only the first is ac-

Table 5. Computation time and noise robustness.

The upper row for each example shows the results for the proposed method and the lower row the results for SDS.

| Example        | Num. of quantities | Num. of data           |               |                |
|----------------|--------------------|------------------------|---------------|----------------|
|                |                    | 50<br>CPU<br>time(sec) | 50<br>Error % | 500<br>Error % |
| Kepler         | 2                  | 2.4<br>10.3            | 5.2%<br>3.4%  | 2.1%<br>2.5%   |
| Heat<br>Trans. | 4                  | 3.6<br>27.7            | 0.5%<br>24%   | 0.4%<br>3.2%   |
| El.<br>Amp.    | 5                  | 4.9<br>74.9            | 8.5%<br>46%   | 4.9%<br>3.7%   |

cepted in the majority of the trials. The robustness against noise is slightly degraded since the candidate target equations are quite complex for the data fitting. The identified equation in the fifth column shows the almost perfect reconstruction of the true target.

The fourth example is the relation among the velocity of a pendulum  $\dot{x}$ , the elapsed time  $t$ , the oscillation angle velocity  $\omega$  and the oscillation amplitude  $A$ .  $t$  which is a ratio scale quantity is commuted to the position of a pendulum  $x$  which is another ratio scale quantity. In this case, the true target equation formula does not match to the candidate since  $t$  and  $x$  have an indirect relation  $\omega t = \arcsin x/A$  where they are coupled with the dimensionless quantities  $\omega t$  and  $x/A$ . In fact, the candidate equation formula was rejected in all  $F$ -tests.

Table 5 indicates some advantages of the proposed method in comparison with the case to discover target equations by a law equation discovery system and check its mathematical consistency with the source equation. SDS is used for the discovery of the target equations. The performances of the proposed method and SDS have been evaluated for the three aforementioned examples under the 5% noise level. The task of the nonlinear least squares fitting occupies the major portion of the computation time of the proposed method because the search space of the reasoning needed to derive the candidate equations is quite limited. The complexity of the nonlinear least squares fitting is  $O(m^2) - O(m^{2.5})$ , where  $m$  is the number of quantities involved in the target equations. This is almost comparable with  $O(m^2) - O(m^3)$  of SDS. However, the actual computation time of the proposed method indicated for the 50 samples case in the third column is far smaller than that of SDS, since the task of the data fitting is the heaviest process, and the required number of the data fitting in SDS is proportional to  $O(m^2)$ , whereas the proposed method performs only once. The fourth and the fifth columns in the table show the error percentage averaged over the

coefficient errors relative to the absolute values of the coefficients in each equation. The proposed method shows very strong noise robustness in case of the larger number of quantities and the small sample data. This is because the noise involved in the data does not affect the reasoning to derive candidate equations. Only the  $F$ -test at the final step can be distorted by the noise. In contrast, the reasoning of SDS can be statistically affected by the noise since the least squares fitting is essentially involved in the reasoning mechanism of the equation formulae. This is a common feature of the conventional law equation discovery systems.

## 5. Application to a Practical Problem

The power of the proposed method is demonstrated through a real world problem in the socio-psychological domain. The objective of the application is to enhance the plausibility of the candidate law equations governing the mental preference of people on their houses subject to the cost to buy the house and the earthquake risk at the place of the house.

In the step (S1) of Table. 3, we designed a questionnaire sheet to ask the preference of the house in the trade off between the frequency of huge earthquakes,  $x_1$  (earthquake/year), and the cost to buy,  $x_2$  (Yen). In the questionnaire, 9 cases of the combinations of the cost and the earthquake frequency are presented, and each person chooses his/her preference from the 7 levels for each case. We distributed this questionnaire sheet to the people owning their houses in the suburb area of Tokyo, and totally 400 answer sheets were collected back. The answer data has been processed by following the method of successive categories which is widely used in the experimental psychology to compose an interval scale preference index  $y_I$  (Torgerson, 1958). The basic principle of this method is to evaluate the quantitative interval distances among the categorical preference levels based on the answer distributions on the categorical levels. The answers on the 7 levels have been transformed to the range of  $[-1.37, 2.04]$  on the interval scale. Hence, a set of observed data  $OBS_I = \{X_1, X_2, \dots, X_{400}\}$  where  $X_i = [x_{1i}, x_{2i}, y_{Ii}]$  is obtained. Because this is a passively observed data set, the original SDS is not applicable. Accordingly, we adopted the extended SDS which can discover law equations from passively observed data (Washio et al., 1999). The extended SDS seeks law equations of the form  $y = f(x_1, x_2)$ , where  $x_1$  and  $x_2$  are ratio scale quantities. The discovered candidate law equations are the following two,

$$y_I = 0.63 \log x_1 + 0.34 \log x_2 - 2.9, \quad (6)$$

$$y_I = -7.9x_1^{-0.23}x_2^{-0.11} + 3.5. \quad (7)$$

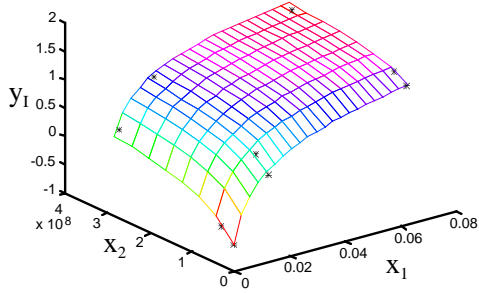


Figure 1. Plot of Eq.(7):  $y_I = -7.9x_1^{-0.23}x_2^{-0.11} + 3.5$ .

The plot of Eq.(7) is depicted in Figure 1. Each black dot in the plots stands for the average point of all cases subject to the cost and the earthquake frequency. Both of Eq.(6) and Eq.(7) fit nicely to the data, and show the monotonic relations among the three quantities.

In the step (*S2*), we designed another style of the questionnaire sheet to ask the identical contents to the same people. In this questionnaire, the preference was asked in form of the paired comparison among the 9 cases of the combinations of the cost and the earthquake frequency. Each person compares two cases at a time, and chooses its relative preference from the 7 levels in each comparison. The answer data have been processed by following the constant-sum method which is also widely used in the experimental psychology to compose a ratio scale preference index  $y_R$  (Comrey, 1950). The basic principle of this method is to evaluate the quantitative ratios among the categorical relative preference levels based on the statistical expectations. The answers have been transformed to the range of [0.04, 12.06] on the ratio scale. Through this process, a set of observed data  $OBS_R = \{X_1, X_2, \dots, X_{400}\}$  where  $X_i = [x_{1i}, x_{2i}, y_{Ri}]$  is obtained. Because both  $y_I$  and  $y_R$  measure the identical psychological feature, they are considered to have the direct dependency. Thus, the commutation of  $y_I$  to  $y_R$  based on the scale-types is applied to both candidates of Eq.(6) and Eq.(7). By substituting 2.1 and 2.2 in Table 2 to the equations, the following four candidate target equations are deduced,

$$y_R = e^{-\frac{\beta_*+2.9}{\alpha}} x_1^{0.63/\alpha} x_2^{0.34/\alpha}, \quad (8)$$

$$y_R = \left( \log x_1^{0.63/\alpha} x_2^{0.34/\alpha} - \frac{\delta + 2.9}{\alpha} \right)^{1/\beta}, \quad (9)$$

$$y_R = e^{-\frac{\beta_*+3.5}{\alpha}} e^{-\frac{7.9}{\alpha} x_1^{-0.23} x_2^{-0.11}}, \quad (10)$$

$$y_R = \left( -\frac{7.9}{\alpha_*} x_1^{-0.23} x_2^{-0.11} + \frac{-\delta + 3.5}{\alpha_*} \right)^{1/\beta}. \quad (11)$$

In the step (*S3*), these equations are subject to the

least square fitting and *F*-test under the data  $OBS_R$ . Only Eq.(8) and Eq.(11) have been accepted by *F*-test, and their resultant equation formulae are as follows,

$$y_R = 0.081x_1^{0.438}x_2^{0.236} \text{ from Eq.(8)}, \quad (12)$$

$$y_R = (1.27x_1^{-0.23}x_2^{-0.11} + 2.46)^{-1.92} \text{ from Eq.(11)}. \quad (13)$$

This fact indicates that both Eq.(6) and Eq.(7) are plausible in terms of the generality over the two questionnaire investigations.

## 6. Discussion

The extended SDS has also been applied to the data  $OBS_R$  obtained from the second questionnaire investigation. The following unique candidate law equation has been discovered by the extended SDS based on the data.

$$y_R = 0.146x_1^{0.449}x_2^{0.207}. \quad (14)$$

The structure of the equation is identical with Eq.(12). Furthermore, their power coefficients are almost the same to each other. This evidence supports the high plausibility of the equations of Eq.(8), Eq.(12) and/or Eq.(14). However, the equation similar to the more complex Eq.(13) has not been discovered by the extended SDS. This may be because the basic algorithm of SDS seeks the law equations starting from the simpler formulae in a bottom up manner. Many of the conventional law equation discovery systems apply similar search strategies taking into account the principle of parsimony. Though this is one of the most important criteria of the first principle law equation, the extra equations meeting with the other important criteria such as the mathematical admissibility and the statistical goodness of fitting are considered to be also plausible, and should be retained in the candidate law equations. In this sense, Eq.(13) should not be missed.

## 7. Conclusion

This paper pointed out the importance of the use of the second generality criterion over multiple combinations of measurement quantities to enhance the plausibility of the scientific discovery. The proposed method based on the admissible relations yielded by the scale-type constraints has the performance of the efficient reasoning, the superior noise robustness and the applicability to the small sample data. These features are highly beneficial since the data acquisition and/or sensing in high quality for the new set of measurement quantities is very expensive in many practical fields. In addition, the ability of the proposed method has been demonstrated to capture the complex but admissible



law equations which may be missed by some conventional law discovery systems as demonstrated in the aforementioned application. Moreover, the ability to detect the indirect dependency between the quantities for commutation has been also demonstrated. Finally, the practicality of the proposed method has been confirmed through the real world scientific law discovery in socio-psychology.

## References

- Comrey, A. L. (1950). A proposed method for absolute ratio scaling. *Psychometrika*, 15, 317–325.
- Dzeroski S., & Todorovski L. (1995). Discovering dynamics: from inductive logic programing to machine discovery. *Journal of Intelligent Information Systems*, 4, 1, 89–108.
- Falkenhainer, B. C., & Michalski, R. S. (1986). Integrating quantitative and qualitative discovery: the ABACUS system. *Machine Learning*, 1, 4, 367–401.
- Koehn, B., & Zytkow, J. M. (1986). Experimenting and theorizing in theory formation. *Proceedings of the International Symposium on Methodologies for Intelligent Systems* (pp. 296–307).
- Kokar, M. M. (1986). Determining arguments of invariant functional descriptions. *Machine Learning*, 1, 4, 403–422.
- Langley, et al. (1987). *Scientific discovery: Computational explorations of the creative processes*. Cambridge, MA: MIT Press.
- Luce, R. D. (1959). On the possible psychological laws. *Psychological Review*, 66, 2, 81–95.
- More, J. J. (1977). The Levenberg-Marquardt algorithm: Implementation and theory. In Watson, G. A. (Ed.), *Numerical analysis: Lecture notes in mathematics 630*, New York: Springer-Verlag.
- Stevens, S. S. (1946). On the theory of scales of measurement. *Science*, 103, 2684, 677–680.
- Torgerson, W. S. (1958). *Theory and methods of scaling*. New York: John Wiley.
- Washio, T., & Motoda, H. (1996). Scale-based reasoning on possible law equations. *Qualitative reasoning: The Tenth International Workshop* (pp. 255–264). AAAI.
- Washio, T., & Motoda, H. (1997). Discovering admissible models of complex systems based on scale-types and identity constraints. *Proceedings of Fifteenth International Joint Conference on Artificial Intelligence* (pp. 810–817).
- Washio, T., & Motoda, H. (1998). Discovering admissible simultaneous equations of large scale systems. *Proceedings of Fifteenth National Conference on Artificial Intelligence* (pp. 189–196).
- Washio, T., Motoda, H., & Niwa, Y. (1999). Discovering admissible model equations from observed data based on scale-types and identity constraints. *Proceedings of Sixteenth International Joint Conference on Artificial Intelligence* (pp. 772–779).